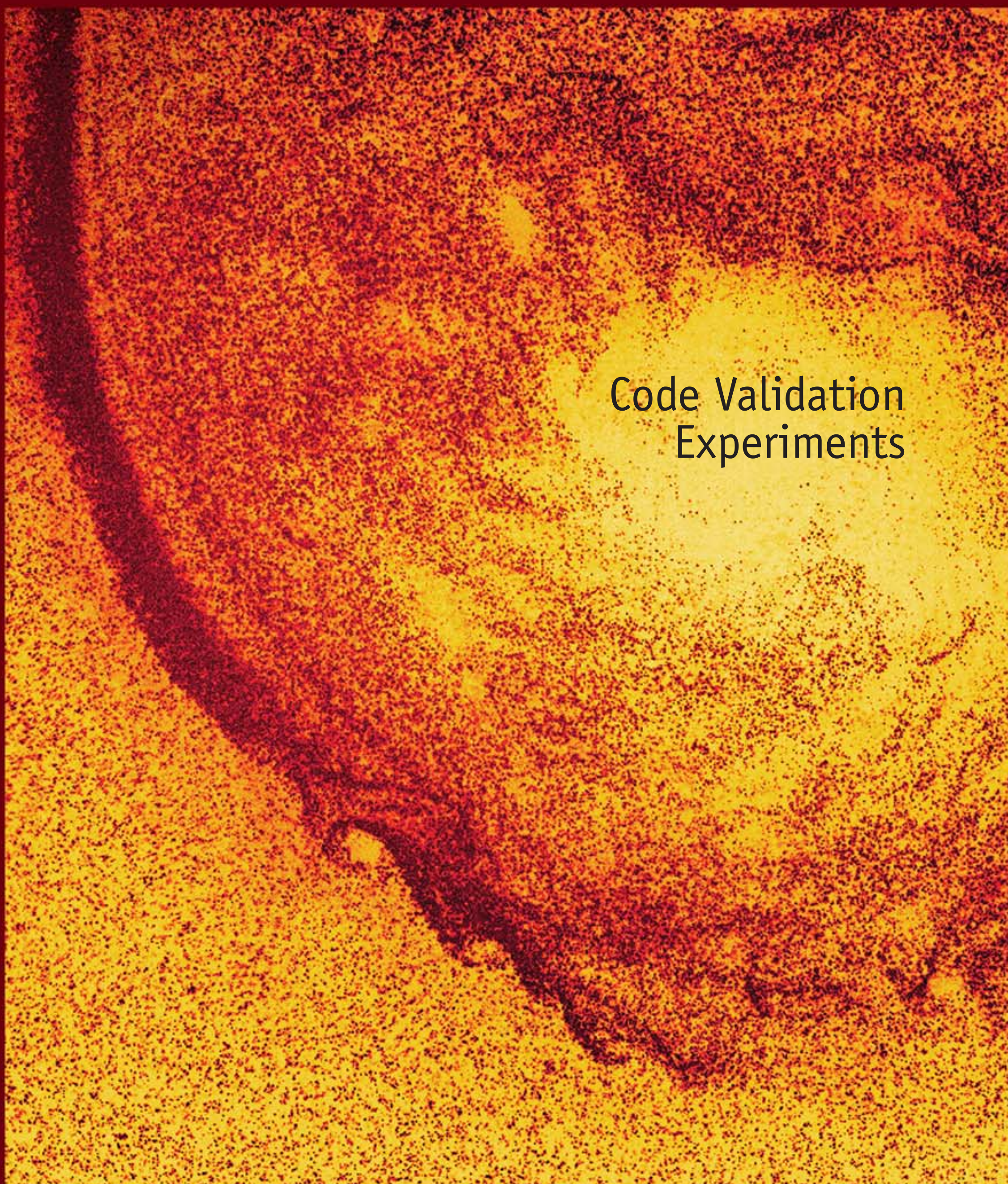
Fall 2002

Los Alamos research QUARTERLY



Code Validation Experiments

Acoustic Tools ▪ Biothreat Analysis ▪ Nuclear Emergency Response

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About the Quarterly

The *Los Alamos Research Quarterly* is published to communicate the Laboratory's achievements and how they benefit our neighbors, our nation, and the world. Operated by the University of California for the Department of Energy and the National Nuclear Security Administration, Los Alamos has a distinguished record of applying science and technology to meet national needs, a record that stretches back to our founding during the Manhattan Project. The *Research Quarterly* highlights our ongoing work to enhance global security by ensuring the safety and reliability of the U.S. nuclear weapons stockpile, developing technical solutions to reduce the threat of weapons of mass destruction, and solving problems related to energy, environment, infrastructure, health, and national security.

Inquiries about this publication should be directed to larq@lanl.gov or to Research Quarterly, Los Alamos National Laboratory, Mail Stop D416, Los Alamos, NM 87545.

About the Cover

The photo on the front cover is a cross-sectional snapshot of one of a pair of vortices formed when a planar shock wave strikes a column of sulfur hexafluoride gas. The field of view is 8 millimeters wide. The "grains" in the image are microscopic glycol/water droplets mixed with the gas in the column and surrounding air to make the gases visible. Because the image is a negative, regions of high gas density are darker than regions of low density. The ripples on the lower edge of the vortex are produced by intense gas swirling, a phenomenon that tests a computer code's ability to model complex fluid flow. The shock-wave experiments are being conducted to validate the codes used to model fluid instabilities and are discussed in the lead article of this issue. The images on the back cover are time-evolution snapshots from an experiment with two shocked gas columns.

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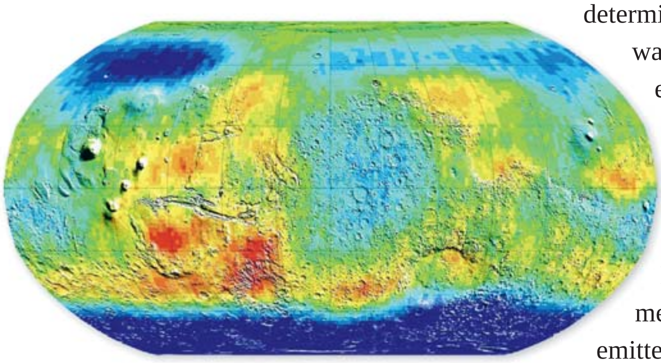
Los Alamos Research Quarterly

Dateline Los Alamos

Mars Odyssey Finds Water



Map of the epithermal neutron flux from Mars—low flux (blue) is indicative of a high hydrogen content.

Los Alamos researchers have determined that Mars has enough water to sustain human exploratory missions. Since February, a neutron spectrometer, designed and built at Los Alamos and flown aboard NASA's Mars Odyssey, has been measuring the neutron flux emitted from the red planet in order to map the global distribution of near-surface hydrogen. The neutron spectrometer is one of three instruments combined in the Mars Odyssey Gamma-Ray Spectrometer, which is operated by the University of Arizona. All three instruments are being used to determine the elemental composition of the Martian surface.

"The surface soils of Mars are rich in hydrogen," said Bill Feldman, the Laboratory's principal investigator for the neutron spectrometer. Soil in the upper and lower latitudes around both Martian poles "contains from 35 to 100 percent of water ice buried beneath a shallow overburden of hydrogen-poor soil. Although scientists have known that water ice is stable close to the surface in these regions, our new measurements are the first to give the amount of near-surface water on Mars," Feldman commented. "We have anticipated these results for 17 years and are excited that all of our wishes and hard work have been fulfilled."

The Lab's neutron spectrometer has been measuring the flux of neutrons

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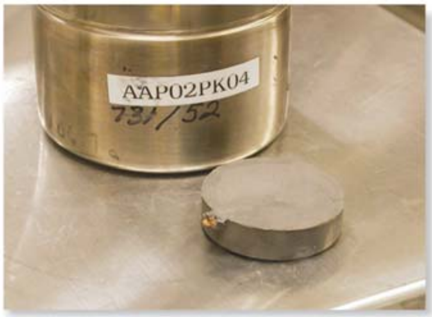
Researchers Cast "Spiked" Plutonium Alloy

In May, Los Alamos researchers cast nine ingots of a "spiked" plutonium alloy and fabricated them into test samples at the Lab's Plutonium Facility (TA-55). The spiking, which enriched weapons-grade plutonium with plutonium-238, created an alloy that should age sixteen times faster than normal. As a result, within four years the researchers hope to have a material representative of sixty-year-old plutonium.



LeRoy N. Sanchez

Researchers cast nine hamburger-sized enriched plutonium ingots like the one shown here.

The much higher radioactive decay rate of plutonium-238 will accelerate the self-irradiation process in the spiked alloy and enhance the resulting radiation damage, such as the formation of helium bubbles and void swelling. Accelerating such aging effects will provide critical data for assessing how radiation damage affects the plutonium cores, or pits, of the nation's nuclear weapons. Detecting and predicting changes in the our aging stockpile are among the more challenging aspects of science-based stockpile stewardship.

"This is probably the most technically difficult project we have ever attempted, at least metallurgically, at TA-55," said J. David Olivas,

continues on page 26

Mesa View

John C. Browne, Director

Richard Robinson

For nearly sixty years, Los Alamos National Laboratory has developed and applied cutting-edge science and technology to critical national security challenges. That work, led by our talented and dedicated scientists and engineers, has sparked significant scientific breakthroughs and technical innovations.

Such service to the nation often lies hidden behind the language of scientific disciplines or the restrictions of security requirements. As a result, the public cannot appreciate the Laboratory's ongoing scientific contributions and how they support national needs in security, health, environmental stewardship, and other areas. I am pleased, therefore, to introduce the *Los Alamos Research Quarterly*, a publication that will highlight our research, introduce the creative people responsible for our achievements, and explain the importance of our programs to national priorities.

Our feature article describes experiments to study how vortices form and interact at the interfaces of different fluids moving through each other. This common event in our everyday world—like cream swirling into coffee, for example—becomes critically important in nuclear weapons, when the fluids are metals driven together under extremely high temperatures and pressures. Our experiments help validate the computational models needed to assess weapon reliability and safety and provide insights into this basic, natural phenomenon.

Another article discusses the use of sound to inspect sealed containers. Subjecting an artillery shell or gas cylinder to a small impulse of sound and analyzing the reverberations can reveal information about its contents, much like listening to a bell's tone reveals its composition. Inspectors now apply this technology to look for deadly biological or chemical munitions.

We also have applied our expertise in analyzing genetic information to categorize strains of the anthrax-causing bacterium *Bacillus anthracis*. By teasing apart an organism's genetic structure, we can identify key features to track its kinship or geographic origin, for example. This expertise supported federal investigations in last year's criminal anthrax attacks.

The publication also offers a look at Los Alamos's support for the Nuclear Emergency Support Team, volunteers drawn from all the national laboratories to provide a national emergency response capability.

Los Alamos ranks alongside the best of the world's scientific institutions because of the excellence and dedication of our staff and our unique experimental and computational facilities. We undertake a multidisciplinary approach to solving complex scientific problems that few other institutions can match—and future advances likely will be made at the intersections of different scientific fields.

At Los Alamos, our emphasis is on use-driven research intended to benefit our society. You will have the chance to read about our work and its benefits in this and future issues of the *Los Alamos Research Quarterly*.

I hope you enjoy what we have to offer you.

Code Validation Experiments

— a key to predictive science

by Brian Fishbine

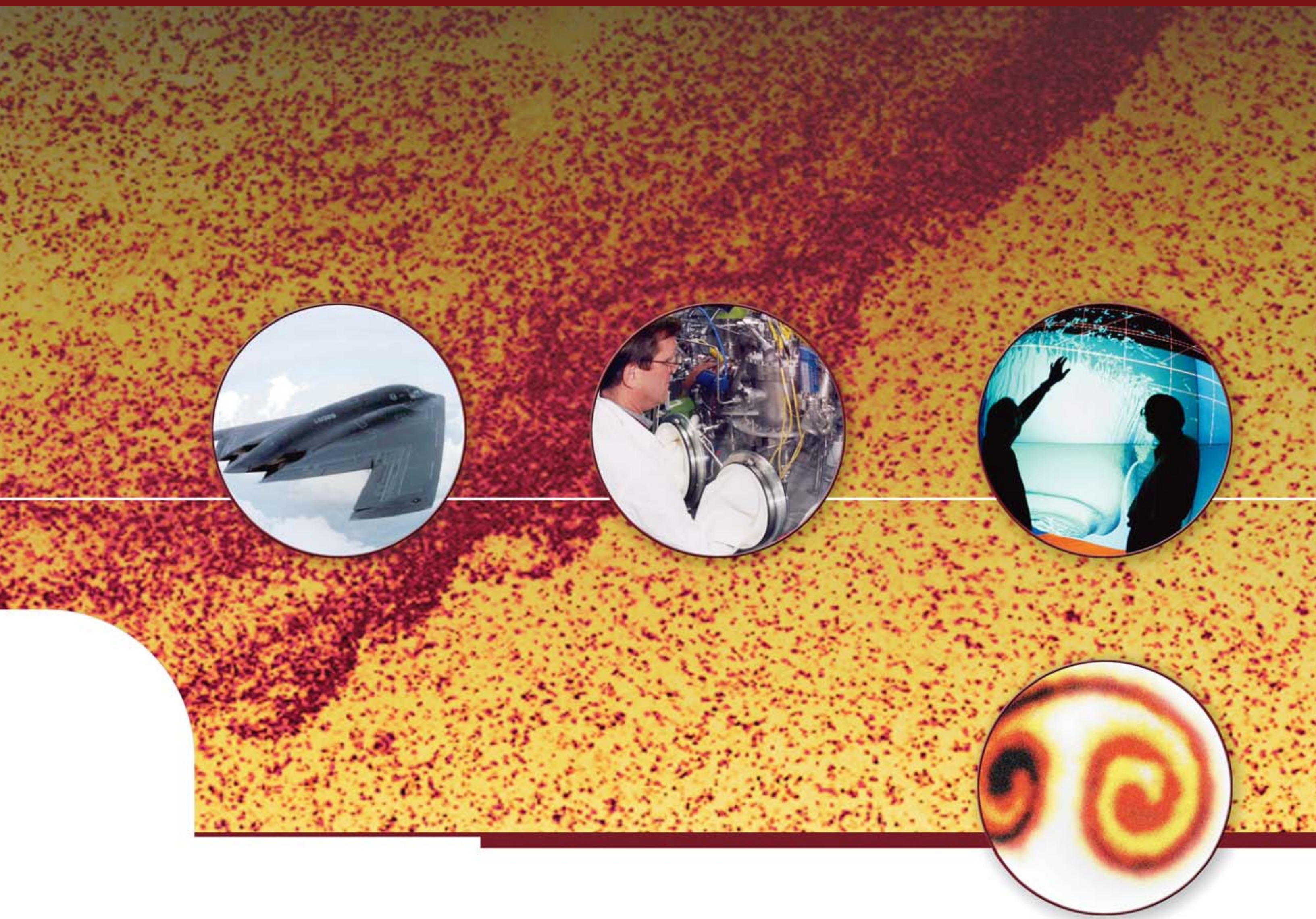
Small-scale laboratory experiments are helping to validate computer simulations of nuclear weapon performance.

The goal of stockpile stewardship—and Los Alamos' core mission—is to ensure the safety, reliability, and performance of the nuclear stockpile. The current ban on underground nuclear testing, however, severely limits the options for carrying out this mission. As a result, we now rely heavily on simulations produced by computer programs, or codes, to predict the performance of a nuclear weapon under various conditions.

Simulations provide far more diagnostic information than a nuclear test does. Using models of the physical processes that occur in a nuclear detonation, a computer can calculate variables such as temperature and pressure for any point in the calculational space of the simulated explosion with high spatial resolution—from the time the virtual bomb goes off (or before) to any time later.

New visualization tools can then present the huge volumes of information produced by a weapon simulation in ways scientists can quickly grasp. (A complete simulation produces nearly fifty times the information contained in the Library of Congress.) For example, one of the new Los Alamos PowerWalls—which each provides a 4- by 2-meter stereo display—can immerse weapon scientists in a full-color, three-dimensional movie of, say, the temperature field of a simulated thermonuclear fireball.

But these stunning displays pose a daunting question: do they show what will really happen? A simulation is only



as good as the equations, algorithms, and computer hardware that go into it, no matter how striking the display. If the computer models are wrong, inappropriate, or incorrectly implemented or executed, the simulation will be flawed—which is unacceptable for stockpile stewardship.

To help ensure that the predictions of weapon simulations are as accurate as possible, experimenters and code users at Los Alamos are using data from a variety of small-scale experiments to validate some of the physics models in the codes. The laboratory experiments discussed in this article focus on one of several fluid instabilities that have been studied by weapon scientists for decades. (Nearly sixty years ago, the Manhattan Project scientists who built the first atomic bomb realized that fluid instabilities could prevent a successful detonation.) However, these small-scale experiments occur at temperatures and pressures far removed from those in a nuclear weapon explosion and use materials quite different from those in nuclear devices. To fully validate a weapon code also requires the use of data from nuclear tests performed before the test ban went into effect as well as data from other experiments, as we discuss later in the article.

Richtmyer-Meshkov Instability

The fluid instability of primary interest in these small-scale experiments is the Richtmyer-Meshkov instability, which occurs when the interface between two fluids with different densities is accelerated by a shock wave

Presley Salaz

New visualization tools such as the Los Alamos PowerWalls help scientists grasp the huge volumes of information produced in a computer simulation of a nuclear explosion. The scientists here are viewing a three-dimensional simulation of a fluid instability. The code-validation experiments discussed in the article produce a two-dimensional version of a similar fluid instability.

striking the interface perpendicularly. The instability was first predicted in 1960 by R. D. Richtmyer, a Los Alamos theorist, and first experimentally observed in 1969 by E. E. Meshkov, a Russian experimentalist.

The instability develops whether the shock travels from a dense fluid to a less-dense fluid or vice versa. For flat or spherical interfaces, the instability causes slight disturbances at the interface to grow into large ripples that breach the interface and mix the fluids. The instability has been observed in inertial confinement fusion (ICF) experiments, in which intense laser or particle-beam pulses heat and compress small, layered metal spheres filled with deuterium and tritium in order to produce fusion reactions. It is also believed to occur in supernova explosions.

Only in recent years, however, have researchers been able to produce the Richtmyer-Meshkov instability in small-scale experiments that yield high-quality data, which is essential for good code validation. Some of these experiments have been performed at Los Alamos by Robert Benjamin and his research team. Related research has also been performed at other national labs, at several universities, and by private industry.

Some of the recent simulations of the Los Alamos experiments were done by Cindy Zoldi, who completed her Ph.D. in applied mathematics at the State University of New York at Stony Brook this past spring, then joined the technical staff at Los Alamos. Zoldi's graduate work involved validating the RAGE code, one of several unclassified codes used to improve physics models through comparison of code results with experimental data.

Gas Column Experiments

In these small-scale experiments, the Richtmyer-Meshkov instability is produced, along with other instabilities, when a planar shock wave propagating in air strikes a small column of sulfur hexafluoride gas, which is five times denser, or heavier, than air. The experiments are designed to produce results that are as two-dimensional (flat) as possible in order to validate the RAGE code in two dimensions. Three-dimensional validation efforts are possible in the future.

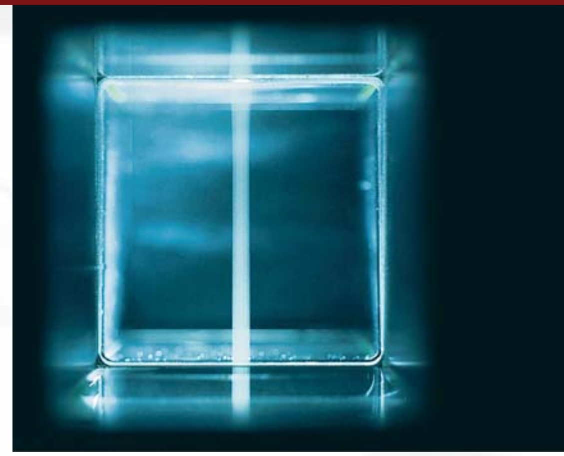
For these experiments the quantities of interest are the gas density and velocity. Seven sequential snapshots of the density show the shock wave first distorting the column of sulfur hexafluoride, then producing finer and finer swirling motion that eventually mixes the gases turbulently. The gas velocity late in the instability's evolution (750 microseconds after the shock wave has left the downstream edge of the column) is also determined from two successive high-resolution snapshots of the evolving column. The velocity is then used to determine the vorticity, a measure of the intensity of the gas swirling.

To measure the gas density and velocity, the experimenters uniformly mix microscopic glycol/water droplets with air and/or sulfur hexafluoride before piping the gas mixture(s) to the experimental chamber. The droplets, generated by a fog machine like those used in theaters for special effects, are about 0.5 micrometer in diameter. Because they're much larger than gas molecules, the droplets scatter light much more efficiently, enabling the gas density to be measured by photographing the brightness of the gas/droplet mixtures. By measuring how groups of the droplets move, the researchers can also produce maps of the gas velocity within and near the shocked gas column.

The gas column is formed by slowly and smoothly piping the dense sulfur hexafluoride through a circular nozzle into the air already present in the experimental chamber. By lighting up cross sections of the column with short laser pulses, the experimenters photographically record the column's density or velocity. Before each laser pulse slices through the gas column, it is spread into a horizontal, fan-shaped sheet about 1 millimeter thick.

The experimenters determine the gas velocity by measuring how far and in what direction groups of the glycol/water droplets move between two successive laser-pulse snapshots. Pattern-recognition software ensures that the velocity is determined for the same group of droplets in two successive frames. Los Alamos was the first to measure high-velocity flow in a shocked gas using this combination of "tracer particles" and pattern-recognition software. The technique was a breakthrough for shocked-gas studies and has greatly enhanced the quality and completeness of the code validation work discussed here.

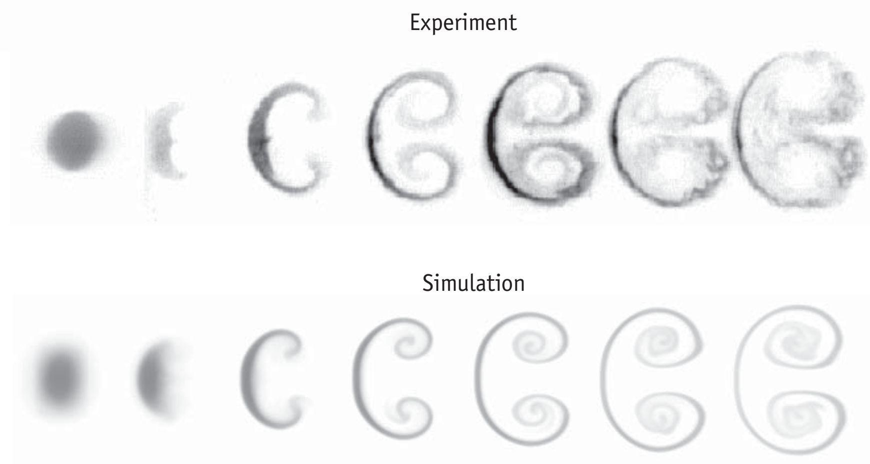
The first section of the shock tube in which the shock wave is generated contains nitrogen pressurized to about three times atmospheric pressure. This section is separated by a polypropylene membrane from a second region of the shock tube that contains air (which is mostly nitrogen) at atmospheric pressure. Rupturing the membrane



Richard Robinson

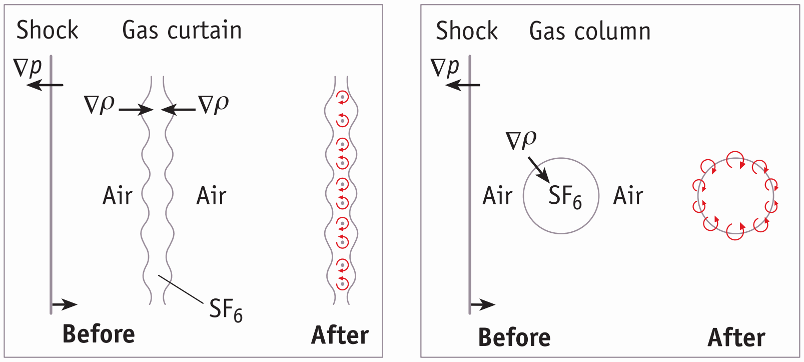
The gas column is formed by piping sulfur hexafluorlde, a gas five times denser than air, through a circular nozzle into ambient air. The column is actually twice the size shown in this photo.

Density Snapshots



Comparison of the experimentally observed and simulated evolution of the shocked column's density. Because these images are negatives, regions of high gas density are darker than regions of low gas density. The initial conditions of the column are shown at the far left; its initial diameter is about 6 millimeters. The shock wave moves from left to right. Time also proceeds from left to right, with 140 microseconds between frames. Time is measured from the moment the shock wave has left the downstream edge of the column. The entire experiment is over in less than a thousandth of a second. Good agreement is seen in the larger-scale structure of the density snapshots. Differences in the smaller-scale structure are the subject of continuing research. Note the pair of large vortices on the downstream side of the shock-wave/column interaction. The core of one of these vortices is used as a reference point for comparing the experimentally observed and simulated velocities late in the instability's evolution.

Vorticity in Shocked-Gas Experiments



(a) (b)

Shocked-gas experiments before and after shock arrival. Vorticity, a measure of the intensity of gas swirling, is a key feature of the complex fluid flow produced by the Richtmyer-Meshkov instability (and other fluid instabilities). Vorticity is produced by the interaction of the incident shock wave's pressure gradient (∇p) with the density gradient ($\nabla \rho$) at the boundary between the sulfur hexafluoride (SF_6) and the surrounding air. The maximum vorticity is produced when the pressure gradient is perpendicular to the density gradient. The schematic compares the vorticity produced in shock-wave experiments with a curtain versus a column of gas. The first shocked-gas experiments of this type at Los Alamos used gas curtains. The directions of the incident shock wave's pressure gradient and velocity are shown by the oppositely directed arrows on the shock front. (a) For a gas curtain, the density gradient points into the curtain at each of its two interfaces. The vorticity distribution just after the shock wave strikes the curtain can be roughly approximated as a row of small, equally spaced vortices of equal size. (b) For the gas column, the density gradient points radially inward. The large vortices at the sides of the shocked column show that much larger values of vorticity are produced for a gas column, which more severely test a code's ability to model complex fluid flow.

abruptly releases the nitrogen into the second region, producing a shock wave with a speed of about 400 meters per second, or 900 miles per hour. Although polypropylene looks like the clear plastic used to wrap food, it has the unique property of shattering when ruptured, making it ideal for generating high-quality shocks.

After leaving the shock generator, the shock wave encounters the gas column formed within the experimental chamber. The chamber has windows through which the laser pulses pass and through which three cameras view the column's initial state and later distortion and breakup.

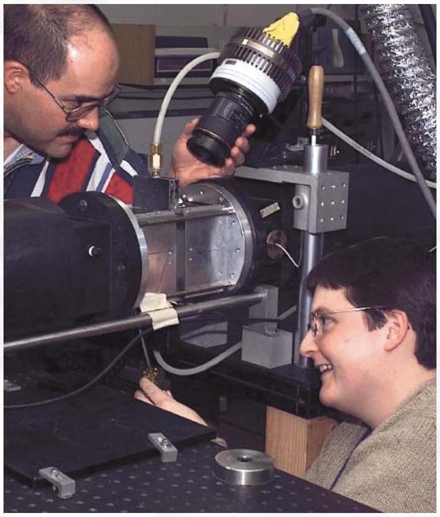
The experiment is fairly compact—the basic apparatus fits on a 6- by 2-meter "tabletop"; the gas column is about 6 millimeters in diameter and 7.5 centimeters tall. However, these small experiments produce big results, as the doctoral dissertations and publications flowing from the research confirm. In addition, four postdoctoral researchers who originally worked in Benjamin's research team were later hired at Los Alamos as technical staff members.

Collaboration is Key

But the validation work has not been easy. Once the experiments began to produce useful data, it took about two years to get the RAGE code results and the experimental data to agree quantitatively. The effort involved close collaboration between the code users and the experimenters—the key to good code validation, says Tim Trucano, a code validation expert at Sandia National Laboratories in Albuquerque, NM. Trucano is a member of the Validation and Verification Program for the Department of Energy's Advanced Simulation and Computing (ASC) program, which involves Los Alamos, Sandia, and Lawrence Livermore National Laboratories. The ASC program, formerly called the Accelerated Strategic Computing Initiative (ASCI), focuses on simulations for stockpile stewardship.

Initially, the simulation showed the shock wave distorting the column generally as seen in the early stages of the experimental shock-wave/column interaction. However, quantitative comparisons of the simulated and experimental results for the distorted column's outer dimensions as functions of time and for the velocity and vorticity fields at a single time were poor. In particular, the simulated peak velocities were about two times larger than the experimentally observed ones.

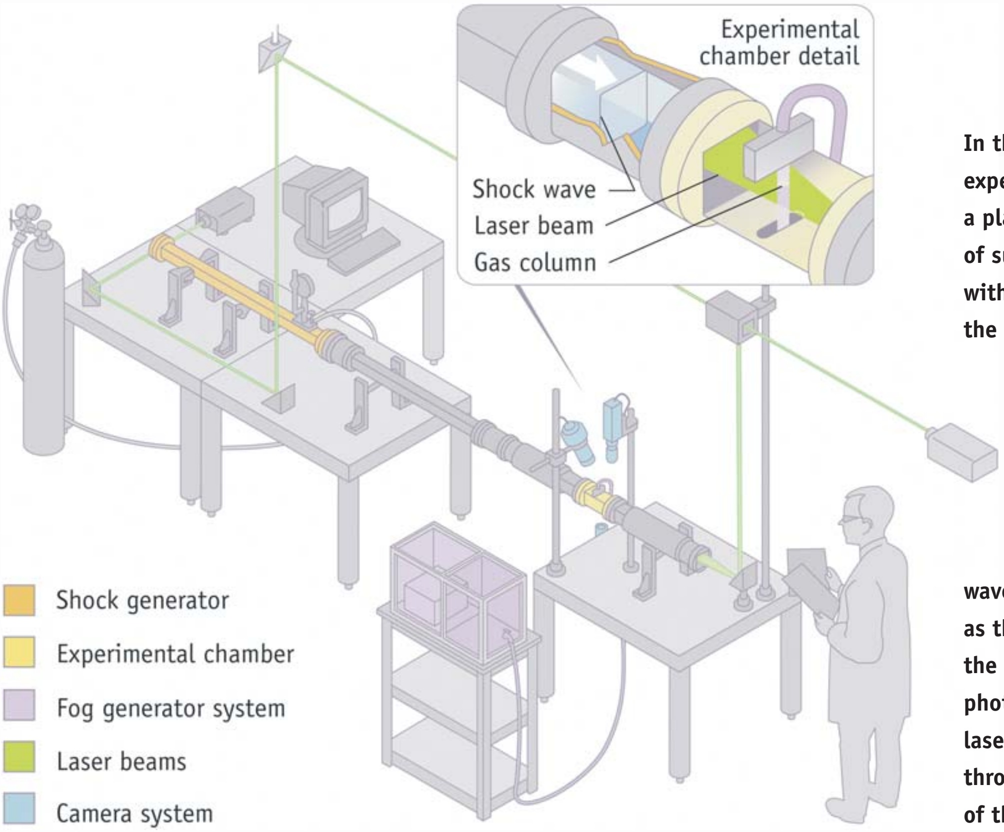
There were several sources of error. For one, Zoldi was able to obtain better agreement with the experiment by using an initial boundary between the sulfur hexafluoride and the surrounding air that was more diffuse than that indicated by initial measurements. Subsequent measurements confirmed that the boundary was indeed more diffuse. In addition, the velocity and vorticity comparisons improved when the experimenters (1) mixed the fog with both the sulfur hexafluoride and



John Flower

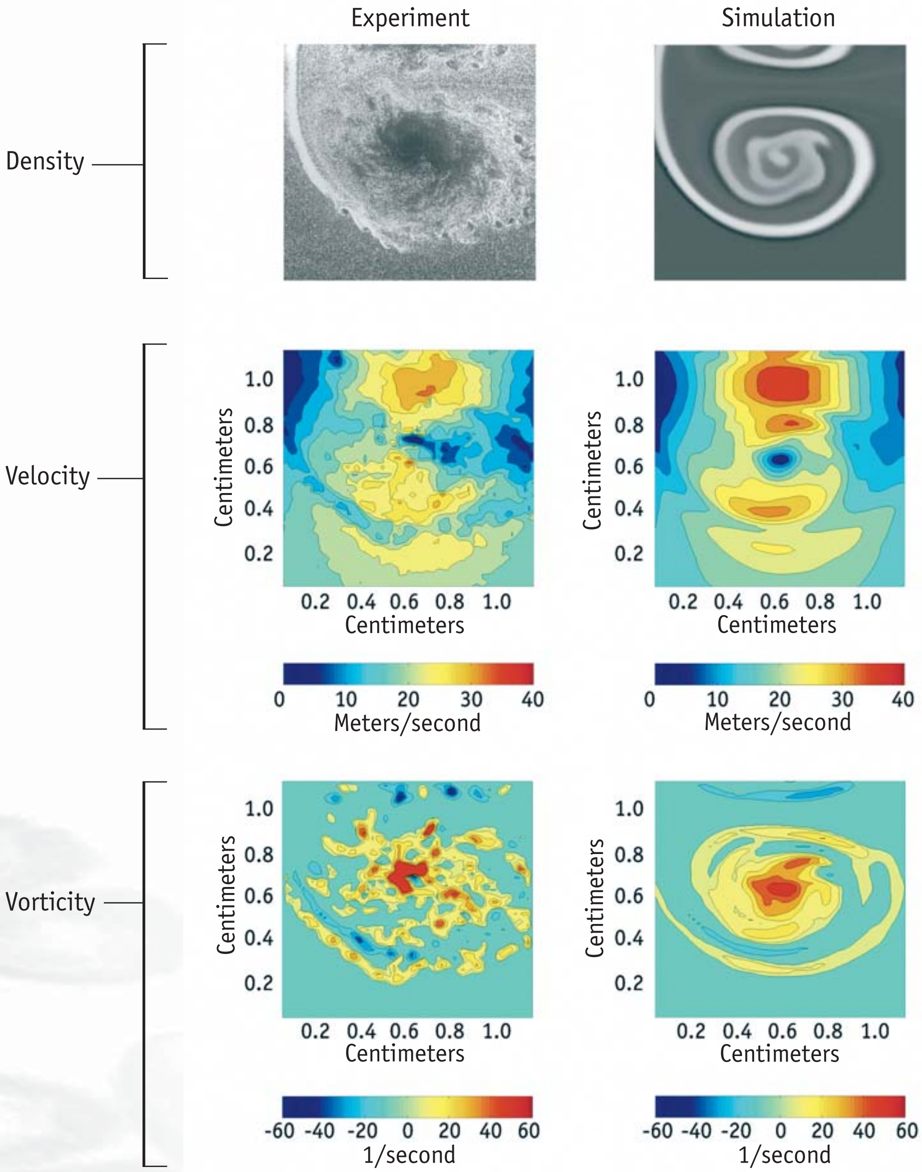
Los Alamos researchers Paul Rightley (left) and Kathy Prestridge (right) prepare to take shocked-gas data that can be used for code validation.

Shocked-Column Experiment



In the gas-column code-validation experiments, a shock generator produces a planar shock wave that strikes a column of sulfur hexafluoride gas formed in air within the experimental chamber. Before the gases are piped into the chamber, they can be separately mixed with a fog of microscopic glycol/water droplets to make them visible. Cross sections of the column's density are photographed before the shock wave arrives and at specific times later as the shock wave distorts and breaks up the column. The light source for these photos is a 1-millimeter-thick pulsed laser beam spread into a fan that slices through the gas column about one-third of the way down.

Experiment and Simulation Comparisons



The experimentally observed and simulated density, velocity, and vorticity for a shocked gas column 750 microseconds after the shock wave has left the downstream edge of the column. After two years of close collaboration between the experimenters and a code user, the experimental and simulated magnitudes of the peak velocities now agree to within 10–15 percent. The signs and magnitudes of the vorticity are also similar for the two cases. As seen in the close-ups of the density comparison, the simulated results reproduce the larger-scale structure of the experimentally observed results but not the smaller-scale structure.

the air to obtain velocity data for both gases and (2) used a higher-resolution camera to take the photos used to measure the velocity.

There was also a problem with the way the predicted and experimentally observed velocities were initially compared. In addition to the large velocity produced by the shock wave's impact, the column receives a small velocity induced by the pair of large vortices generated in the shock wave's wake. The effect of this added velocity had not been taken into account. When it was, together with the other improvements, the experimental and simulated values for the fluid's peak velocity agreed to within 10–15 percent. The various fixes substantially improved the velocity comparison.

In Trucano's view, this work is a perfect example of the give and take between experimenters and code users that is required for good code validation. And the collaboration paid off with good agreement between the simulation and the experiment for the larger-scale structure. But at present the RAGE code cannot reproduce the later experimental phases when submillimeter ripples form that lead to turbulent gas mixing. The ripples are quite clear in the laser-pulse photos (see cover photo, for example) but not in the simulations.

A major purpose of code validation is in fact to determine the ranges of experimental parameters for which the code produces accurate results. (It's not mathematically, physically, or economically possible for a code to exactly reproduce the experimental results.) For this particular experiment the code is now valid for the larger-scale structure, although efforts are ongoing to reproduce the fluid's late-time smaller-scale behavior as well.

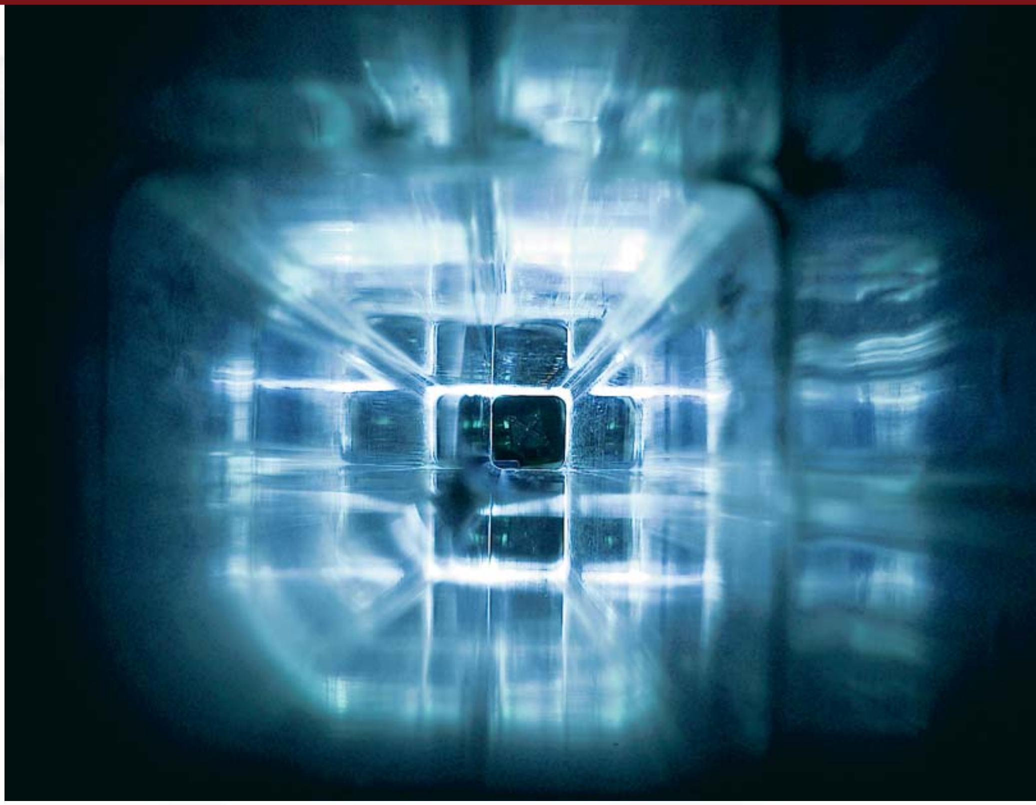
Although the agreement obtained thus far gives confidence in the code's ability to correctly model complex fluid flow, the validation technique itself can be made even more quantitative. Other Los Alamos researchers are using advanced mathematical tools—fractals, wavelets, and structure functions—to quantitatively compare the simulated and experimentally observed complexity of the turbulent fluid's late-time structure. Their research is at the forefront of the new science of code validation.

Regarding the importance of using experiments to validate codes, Los Alamos Director John Browne says, "Code-validation experiments are the foundation of predictive capability."

Other Validating Data

In fact, weapon code users at Los Alamos currently use data not only from small-scale experiments like Benjamin's but also from nuclear tests performed before the Comprehensive Test Ban Treaty went into effect and from a variety of large-scale experiments as well, including hydrotests, subcritical tests, and magnetic-compression and ICF experiments.

Hydrotests help code users interpret the results of some codes that simulate the implosion of a nuclear weapon. During implosion, shock waves produced by high explosives compress nuclear materials to supercritical mass. (The term hydrotest comes from the fact that, during implosion, the high pressures and temperatures generated by the high explosives cause metals and other materials to flow like liquids.) By imploding nonnuclear surrogate materials with properties similar to



Richard Robinson

Internal reflections produced this kalaidoscopic image of the shock tube used in the shocked-gas experiments. The end of the tube, whose internal dimensions are 7.5 by 7.5 centimeters, is the small black square at the center.

The Researchers

Robert Benjamin received a B.S. in engineering physics from Cornell University and a Ph.D. in physics from M.I.T. Since joining the Lab in 1973, he has done x-ray and optical imaging for ICF experiments, developed diagnostics for pulsed magnetic-compression experiments, and conducted fluid-instability experiments. Benjamin received the 1994 Los Alamos Fellows Prize for outstanding research and became a Laboratory Fellow in 1997. He has three patents and over thirty publications.

Cindy Zoldi received a B.S. in electrical engineering from the University of Maine and an M.S. and Ph.D. in applied mathematics from the State University of New York at Stony Brook. She joined the Lab in 2002 as a technical staff member. A member of the Society for Industrial and Applied Mathematics, the American Physical Society, and the Association for Women in Mathematics, Zoldi has presented her research on fluid instabilities at various national and international conferences.

those of nuclear materials, hydrotests simulate weapon implosion without producing a nuclear explosion. In contrast, data on nuclear materials without implosion is obtained from subcritical tests performed at the Nevada Test Site.

At present, Los Alamos has two hydrotest facilities. PHERMEX, the Lab's hydrotest workhorse for nearly forty years, takes x-rays of implosion from a single direction at two times. When fully operational in 2004, the second facility, DARHT, will take x-rays of implosion from two perpendicular directions at up to four times.

More recently, protons instead of x-rays have also been used to image implosions. Proton radiography has the potential to take tens or hundreds of images per hydrotest, providing implosion movies and possibly three-dimensional images as well. Using protons produced by the 800-million-electronvolt accelerator at the Los Alamos Neutron Science Center, preliminary proton-radiography experiments are being used to test concepts for "advanced hydrotest imaging."

Ranging from small shocked-gas experiments like those in Benjamin's lab to large hydrotests, a wide variety of experiments are providing the data scientists need to validate the physical models in the weapon codes. John Browne puts the importance of code validation in a national perspective. In a statement to Congress this past June, he observed that a major component of the stockpile stewardship mission is "predictive science," which will allow the weapons complex "to evaluate how any issue in the stockpile, or any change that we might consider, will affect system safety, reliability, and performance." ■

Code Validation and Stockpile Stewardship

By Ray Juzaitis, Associate Director, Weapons Physics

The goal of stockpile stewardship is to ensure that the weapons in the enduring nuclear stockpile, both today and in the future, are safe and reliable and will perform as expected—including those weapons that may have undergone changes due to aging, refurbishment, or other required modification. To meet this goal, we must sustain our existing expertise in weapon physics, engineering, and manufacturing, as well as sustain the technologies and facilities that support our mission. To meet the challenge potentially posed by future changes in requirements, we must also explore and develop new expertise and new support capabilities.

Because stewardship activities must occur without nuclear testing, we now rely heavily on computers to simulate nuclear weapon performance. Indeed, some of the most powerful computers and computer programs in existence are currently used to assess, in astonishing detail, the performance of complete nuclear weapon systems.

But decisions about the stockpile based on simulations will be well founded only if the simulations' physical models are validated with experimental data. The accompanying article describes validation work at Los Alamos that draws on data from elegant and precise small-scale experiments with shocked gas columns. These experiments are helping us explore and understand hydrodynamic instabilities, which play a significant role in nuclear weapon performance. These experiments also provide an excellent example of the experimental science needed to validate the simulations upon which stockpile stewardship vitally depends.

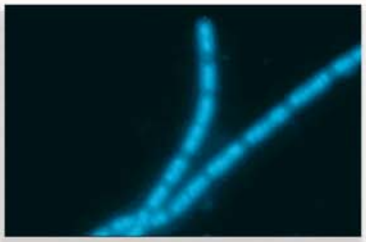
Tracing Biothreats

with Molecular Signatures

by Amy Reeves

Fragments of anthrax DNA in gel

Biological agents have long been used as tools of war and terrorism. Unfortunately, today's biological weapons are far more sophisticated than the plague-infested corpses catapulted over city walls or the dead livestock used to poison medieval water supplies. A few nations have devoted considerable resources to "weaponizing" and stockpiling infectious microbes.



Stained *Bacillus anthracis*

Bacillus spores

Photos by Kevin N. Roark

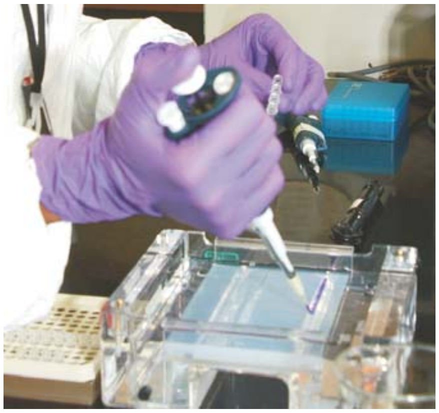
For over a decade, a team of researchers in the Bioscience Division has been working to prevent the proliferation of biological weapons. The team has developed a powerful set of tools and techniques for deciphering molecular signatures—genetic patterns that distinguish bacterial species and strains. These signatures are key to detecting, identifying, and tracing potential biothreat agents, including the microbes that cause anthrax, plague, and botulism.

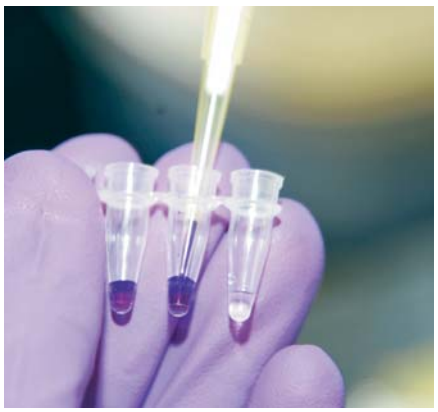
DNA Extraction and Analysis Tools

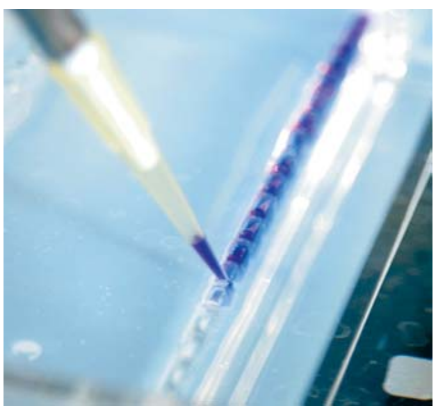
Some of the team's tools, such as rapid DNA-sequencing and bioinformatics techniques, were originally developed as part of the Human Genome Project. Others were developed to solve specific problems encountered during the team's early efforts to devise ways to detect DNA from biothreat agents in environmental and forensic samples.

The first problem was how to extract the DNA to be analyzed. The team devised new methods and instruments to wrest enough quality DNA from preserved tissue or complex environmental samples (such as from soil, ventilation filters, or liquid waste streams) to allow detailed molecular analyses.

The researchers then had to develop a method to determine whether the extracted DNA included DNA from any known biothreat agents. The method had to be sensitive enough to detect trace amounts of biothreat DNA and, to avoid "false positive" results, specific enough to detect DNA only from such







Photos by Kevin N. Roark

(Top) Samples of anthrax DNA are loaded into a gel. Gel electrophoresis is used to separate DNA fragments for analysis. (Middle) Close-up of fluorescent dye being added to DNA samples before they are loaded. (Bottom) Close-up of the gel during loading. The separated fragments (shown in the gel on page 15) provide information about the anthrax strain and its likely sources.

agents and no others, including any close relatives.

Most samples, whether medical or environmental, contain a "mishmash" of DNA from all the organisms or tissue collected, such as human DNA in medical samples or benign soil bacteria and decomposed leaf remnants in environmental samples. The researchers realized that to identify specific DNA from this mishmash, they had to make the target DNA "stand out." The detection method they developed, which is now used by the FBI and the Centers for Disease Control, uses PCR, or polymerase chain reaction, to amplify (make more copies of) the target DNA.

PCR is a laboratory technique that mimics nature's method for replicating DNA. During natural DNA replication, after enzymes unzip the complementary strands of DNA, other enzymes, called polymerases, use the single strands of DNA as templates for producing new complementary strands. The result is two DNA helixes formed from one. The PCR technique uses short DNA fragments, called primers, that bind to part of a strand of target DNA and provide a starting point for the DNA polymerase. After the target DNA has been copied, the strands are separated, and the process

Anthrax Investigations

In 1979, an outbreak of anthrax in the Soviet Union killed more than sixty people. Soviet officials attributed the outbreak to consumption of contaminated meat. However, Western scientists suspected the real cause of the outbreak was inhalation of spores accidentally released from a nearby military research facility.

When the Bioscience Division team analyzed the DNA in preserved tissue samples from eleven victims, it found that the victims were infected with at least five separate strains of *Bacillus anthracis*—in contrast with all known natural outbreaks, which involve a single strain. The multistrain infections suggested that the Soviets were intentionally mixing strains, possibly to complicate initial identification or to experiment with multiple-drug or vaccine resistance.

During an investigation of Iraq's suspected biological weapons program, agents from the United Nations Special Commission (UNSCOM) collected samples from several research and production facilities, including one at Al Hakam. Iraq claimed this facility produced only animal feed and pesticides for agricultural crops. However, the Los Alamos team's molecular analyses detected genetic signatures from an organism that was closely related to *B. anthracis* and somewhat related to the biopesticide *B. thuringiensis,* though it lacked any pesticide properties. The large quantity found in samples collected from an industrial-scale drying unit raised the possibility that the organism was being used as a surrogate for *B. anthracis*.

is repeated until there are enough copies of the target DNA for analysis.

The PCR primers developed by the Los Alamos team are key to the specificity of its detection method. To bind to the template strand of target DNA—a prerequisite for PCR amplification—the primer must be complementary to part of the target DNA. By creating a set of primers with DNA sequences specific to each biothreat agent, the team developed a way to unequivocally amplify only DNA from specific pathogens.

Beyond Species: Identifying Strains

Because all potential biothreat agents are derived from natural sources, determining where a microbe came from and whether or not it was introduced by human activities requires more-detailed analysis. The approach pioneered by the Los Alamos team and their collaborators at Northern Arizona University has been to study the molecular genetics of different pathogens beyond the species to the strain level. The team has developed a battery of methods for distinguishing strains based on tiny differences in their DNA sequences. These methods can even reveal whether a strain has been genetically engineered to complicate identification or enhance drug resistance.

One widely used method relies on enzymes to break the microbe's DNA at specific places. The pattern of the sizes of fragments generated—the fragment profile—is then compared with profiles in a database. If it exactly matches a profile in the database, the microbe's identity can be determined, as well as where the microbe may have originated and how it might be treated. If the profile does not exactly match another but shows significant similarities, scientists can at least determine the microbe's relationship to other species and strains.

Other methods use strain-specific PCR primers to magnify subtle differences in the DNA sequences of related strains. Such primers are already available for the microbes that cause anthrax and plague, and the team is working to design strain-specific primers for other species.

And still other methods involve determining and comparing DNA sequences. Sequence data enables scientists to verify the identification of a species or strain, and it provides clues about how the microbe works—for example, why one strain might be more infectious or more resistant to an antibiotic than another.

Given its expertise and diagnostic tools, the team has been asked to provide technical support to several international investigations involving suspected biological weapon programs (see the sidebar on page 16). "Our strong foundation in biology and genetics has enabled us to respond rapidly when called upon," explained Jill Trewhella, Director of the Bioscience Division.

Los Alamos is also providing technical support to several ongoing investigations, including the response to last fall's anthrax attacks. These attacks caused five deaths, as well as widespread fear, and had significant economic repercussions. A larger attack—whether directed at humans or key agricultural crops—could be even more devastating. "Our hope is that our detection, identification, and attribution expertise will deter the use of such weapons," Trewhella continued, "and that anyone tempted to use such weapons will realize that if they do, we will identify them and they will be caught." ■

Photo courtesy of The White House

During a recent DOE demonstration on homeland security, Bioscience Division Director Jill Trewhella briefed President George W. Bush on Lab technologies for analyzing DNA from biothreat agents. Trewhella showcased the Lab's "dirt to data" portable DNA analysis system, which extracts and quantifies DNA from environmental samples, amplifies target DNA through the use of PCR, and analyzes the results. She explained how the division's research supports national security: division scientists have quickly leveraged technologies developed for programs such as the Human Genome Project by adapting them to analyzing biothreat agents.

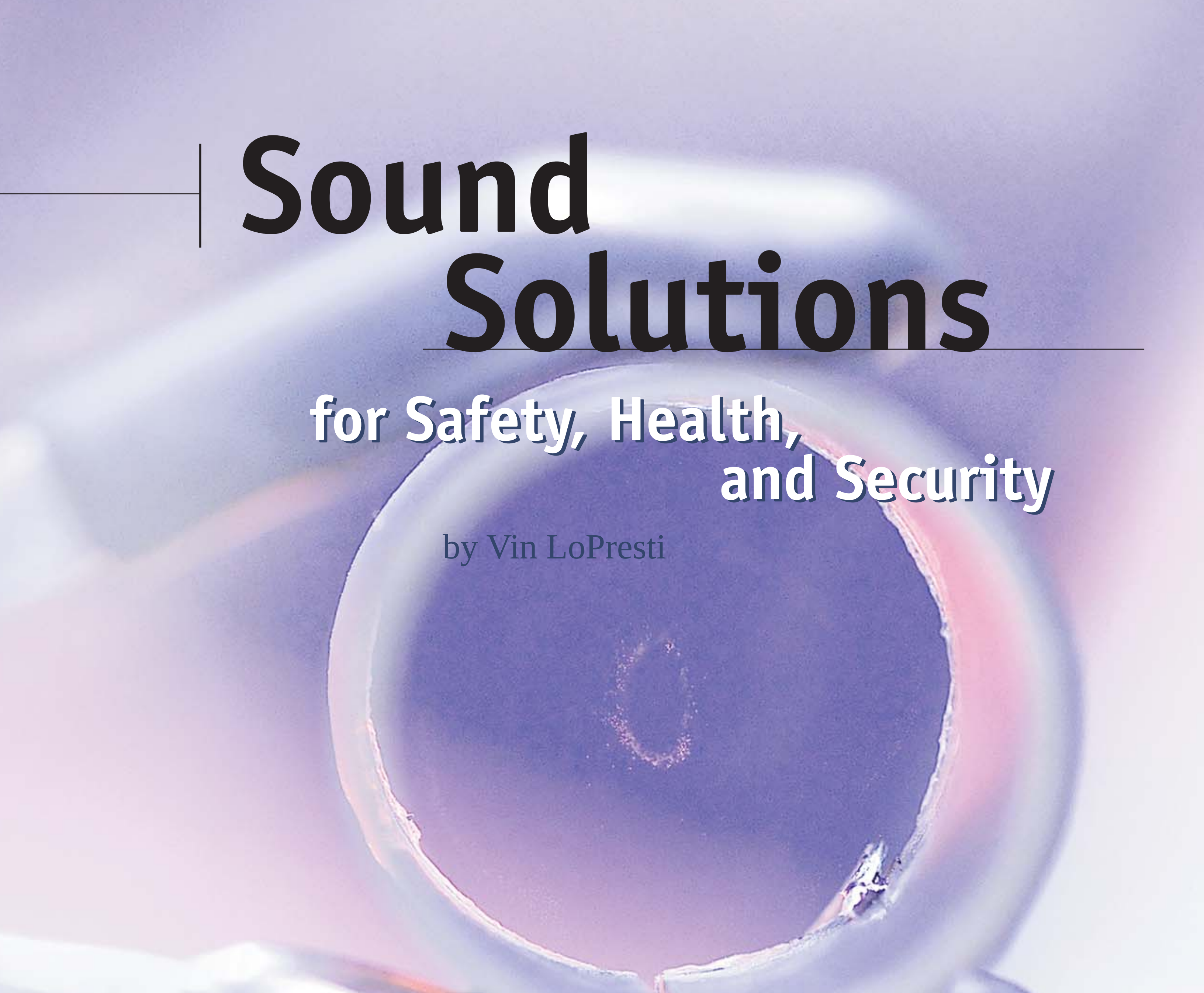
The Researchers

Over its history, the **Bioscience Division team** has included scientists from a variety of disciplines across the Laboratory. From the beginning, the team has been led by **Paul Jackson**, who joined the Laboratory in 1981 after earning his Ph.D. in molecular biology at the University of Utah. Jackson holds six patents and is a Laboratory Fellow.

Sound Solutions

for Safety, Health, and Security

by Vin LoPresti



Sound pressure generated by an acoustic concentrator levitates a ring of aerosol droplets.

Finding out what is in a closed container can be a daunting task when you can't open it—either because its contents may be toxic or because it is someone else's property.

"Why not just tap and listen?" Dipen Sinha once suggested to a group of government officials gathered to assess ways to verify compliance with the 1990 U.S./Soviet Union Chemical Weapons Treaty. Requiring only a metal key, his simple strategy was nonetheless effective.

Since formalizing that idea by developing a sound-based tool for noninvasive fluid identification, Sinha has assembled a team of talented scientists and technicians, inventors who seem capable of devising endless uses for sound. With backgrounds in theoretical physics, chemistry, engineering, and hardware and software design, this versatile team has tackled such questions as "is this food fit to eat" and "where are the best oil deposits?" From answering "what's in the drum" to "what's in your blood," the team's sonic sniffers promise continued solutions for practical problems.

Background photo by Alistair Neal

Sound as Pressure

Underpinning many of the team's inventions is the basic science of sound as pressure waves (see the sidebar on wave phenomena). The vibrations of a loudspeaker inform us that its speaker cone is intermittently pushing (exerting a force on) the surrounding air. Such intermittent pressure on air molecules sets them into wave motion. That motion subsequently vibrates your eardrums, the first step in sound perception.

But high-frequency sound pressure can also be applied to microscopic structures—cells, viruses, and the molecules in a broad range of liquids and gases. The team's specialty is devising ways of carefully controlling sound pressure to use it either as a probe for identifying the contents of closed containers or as a microscopic mover, capable of concentrating airborne or liquid-borne particles to facilitate their analysis.

Many of the team's inventions rely on the positive reinforcement of sound-pressure waves to generate larger-amplitude waves—the phenomenon of resonance or "standing waves." Church bells in a carillon exemplify this acoustic phenomenon. Differing in size and often in thickness, bells not only produce a characteristic frequency (pitch) when struck, but they continue to resonate with one or more frequencies thereafter. Each bell's unique characteristics as a sound conductor define the frequencies that reinforce one another, thus setting up standing waves, which we hear as a bell's lingering reverberation.

Sound Signatures

When the physical properties of a container's contents are unknown, the technique of swept-frequency acoustic interferometry can reveal them and be used to characterize the contained substance(s). By generating sound waves of many different frequencies (sweeping the frequency) and introducing them, one at a time, into the wall of the container, an investigator can empirically discover the characteristics of the container's wall and its liquid-filled cavity.

Because liquids differ in properties such as the speed at which they conduct sound and how much they absorb sound waves, a container's contents affect sound-wave transmission, which consequently exhibits peaks at certain frequencies. The contents thus "pick out" their own resonant frequencies. The resulting spectrum of standing waves superimposes two sound signatures—one for container's wall and one for its contents. This "resonance spectrum" is monitored by a sensitive detector, and mathematical relationships are used to extract properties such as liquid sound speed, sound absorption (attenuation), and density. When compared against a database of acoustic signatures, the properties derived from the resonance spectrum can identify a container's contents.

In addition, by improving on existing sound-projection technology using carrier waves, the team can introduce its resonance-probing sound waves into a container from distances of up to 15 feet. When containers may enclose highly toxic or inflammable substances, such standoff diagnosis is clearly desirable.

One of many acoustic techniques whose development was sponsored by the Department of Defense, acoustic interferometry also has medical applications. An example is diagnosing arthritis or osteoporosis by comparing the acoustic characteristics of diseased joints and bone with those of their healthy counterparts. Novel applications

Wave Phenomena

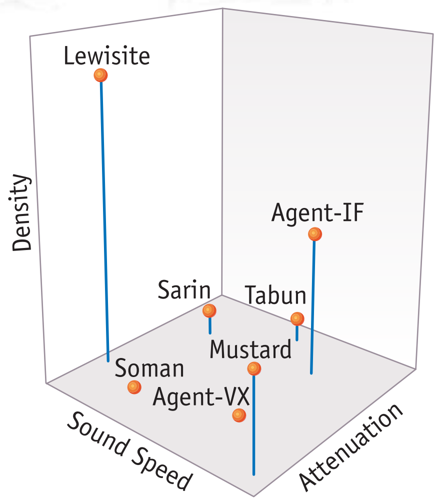
Drop a pebble into a pond, and the disturbance will produce ripples on the surface. If you float a scrap of paper at one point on the ripple (wave) pattern, the paper will bob up and down as "surges" of water molecules intermittently push on the paper's underside. Each surge represents a momentary increase in pressure. Sound waves use air molecules as the "pushing medium," and analogous surges and decreases in pressure occur.

are likewise anticipated as sound projection techniques continue to improve. For example, using sound pressure to launch decontaminating vapors could help to sanitize buildings, a need illustrated by the massive post-9/11 effort required to decontaminate the U.S. Senate offices of anthrax.

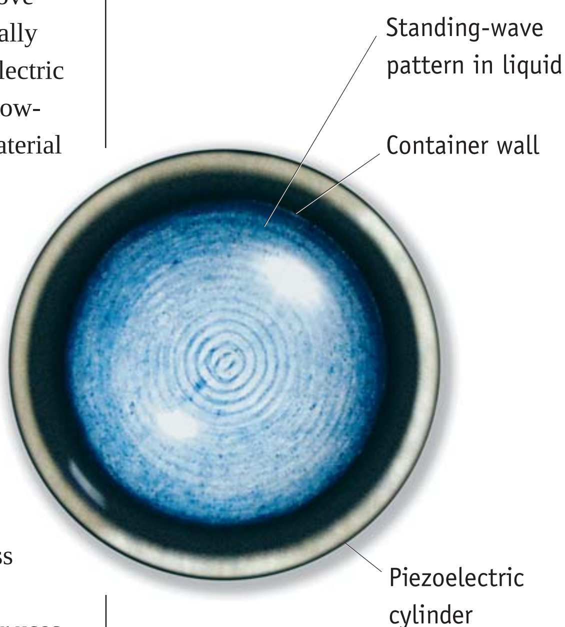
Corralling Particles with Sound: Acoustic Concentrators

Sound pressure and resonance also combine in the functioning of acoustic concentrators. Using sound to move particles, concentrators are basically small hollow cylinders of piezoelectric material. When stimulated with low-power alternating voltage, the material changes shape and intermittently pushes on any air or liquid contained inside the cylinder. These pressure surges create standing waves in that internal medium, which force the enclosed molecules into a set of concentric rings. Air or liquid molecules and any suspended contaminants are more concentrated within the rings, less concentrated between them.

A liquid acoustic concentrator uses resonant sound pressure to move particles suspended in fluids that are contained within the cavity of a cylindrical transducer (a cylinder of piezoelectric material that converts electrical signals to sound pressure). The cavity's resonance frequency changes as the particles are concentrated. An investigator can query the liquid inside the concentrator about its particle content by observing how the cavity's resonance changes as a function of time. For example, a friendly yogurt bacterium like acidophilus differs in size, shape, and other physical properties from a food-spoiler like salmonella or a lethal bioterrorist agent like anthrax, and so its influence on the liquid and how it concentrates under sound pressure will also differ. Friend can thus be distinguished from foe within a few seconds of examining a container suspected of bacterial contamination.



Dr. Sinha uses acoustic interferometry to distinguish chemical weapons from standard artillery shells. Many common chemical warfare agents—such as the ones shown here—can be uniquely identified by comparing three parameters derived from resonance-spectrum data: liquid density, sound speed, and sound attenuation.



Example of the standing-wave pattern that develops in a liquid after sound stimulation with an acoustic concentrator. Blue particles are more concentrated in the concentric blue rings, less concentrated in the lighter-colored spaces between. This diagnostic tool can be used to examine containers of varying sizes.

This technique builds on previous success in which acoustic methods were used to detect the presence of salmonella contamination in unbroken eggs. Nor are acoustic concentrators limited to threat reduction. Applied slightly differently, resonant sound pressure can become a concentrator of blood, gently separating cells (the suspended particles) from plasma (the liquid).

The team has also devised an aerosol acoustic concentrator capable of concentrating airborne contaminants fifty to a hundredfold. Inserting this simple, inexpensive device into the inlet of portable air monitors—such as those that would be used to screen a workplace for anthrax contamination—boosts contaminant-detection sensitivity by that same fifty to a hundredfold, making it less likely that potentially lethal contaminants will escape detection.

Raising a Flag

Recently, the team has expanded its repertoire of threat-detection tools beyond strictly acoustic ones. Suppose you're in charge of airport security and need to rapidly screen passengers to narrow the field of candidates for more detailed searches. You might find use for a fifty-dollar dielectric sensor developed by the team. Held close to beverage or food containers, the sensor will, with the click of a button, unobtrusively establish whether they contain a benign water-based liquid or a possibly explosive hydrocarbon like gasoline.

By sending an electromagnetic pulse into the liquid and measuring the capacitance of a circuit that includes container and contents, the sensor assesses the liquid's dielectric property—its ability to store charge and potentially conduct a current. As anyone knows who has been ordered out of a swimming pool during a thunderstorm, water is a good electrical conductor. Hydrocarbons, however, are not. If a passenger's response to a polite inquiry about a container's contents ("it's baby food," for example) did not match the sensor's response, you might justifiably pursue a more comprehensive search.

Ubiquitous Applications

What is remarkable about Sinha's team is its ability to see a host of problems that could lend themselves to variations on its technologies and then to respond by devising an invention. For example, the team is currently engaged in discovering solutions to such problems as imaging breast cancer without exposing women to the high-energy radiation involved in mammography, monitoring blood-sugar levels without the need for needle sticks, noninvasively determining whether a shipping container has been tampered with, and remotely detecting structural defects in natural-gas pipelines without interrupting delivery to consumers.

The team's contribution to safety, health, and security is evident in each of these envisioned sound solutions. And with prospects for combining many of its inventions into suites of progressively more useful tools, the sounds seem destined to grow only sweeter. ■

Alistair Neal

Dielectric sensor gives a positive indication (red light) that this liquid is water based.

The Researchers

Dipen Sinha received a Ph.D. in physics from Portland State University, after undergraduate and graduate education in India. He holds twelve U.S. patents with several more pending and has received three R&D 100 Awards.

Greg Kaduchak received his Ph.D. and M.S. in physics from Washington State University and a B.A from Saint Louis University. He is a recent recipient of the FBI Director's Award and an R&D 100 Award.

Chris Kwiatkowski received his Ph.D. and M.S. in physics from Washington State University and a B.S. from the University of Toledo. In addition to acoustics, his research interests extend to optics and digital signal processing.

Other team members include Dr. Kendall Springer, Dr. Alexander Kogan, David Lizon, and Greg Goddard.

Render Safe

Defusing a Nuclear Emergency

by Eileen Patterson

The extra duty is inconvenient and could turn dangerous, but Los Alamos staff volunteer because it serves national security and because their expertise is rare: they know the ins and outs of nuclear weapons like few others in the world.

Jose (Mitzie) Ulibarri

At a simulated crash site, Accident Response Group members plan how to secure a nuclear weapon (the cylindrical object in the wreckage). A plane crash involving a U.S. nuclear weapon is unlikely since the cessation of frequent airborne alerts, but ARG volunteers train for all possibilities.

A Shield against Disaster

A number of scientists, engineers, and technicians at Los Alamos are volunteers on the Nuclear Emergency Support Team (NEST), a Department of Energy (DOE) team that is always on call as the nation's shield against a nuclear weapon emergency. Two of the NEST branches staffed by Lab volunteers are the Accident Response Group (ARG), which would deal with an accidentally damaged U.S. nuclear weapon, and the Joint Technical Operations Team (JTOT), which would respond to the threat of a terrorist device. In this work, Los Alamos joins other DOE facilities, including Lawrence Livermore and Sandia National Laboratories.

Beyond their full-time jobs, Los Alamos NEST volunteers serve their on-call duty in rotating one-week shifts. During that week, they keep their equipment packed and stay no more than a few hours' travel time from Kirtland Air Force Base in Albuquerque, a short leash that restricts family activities. Their pagers could sound at any time, but for now, the calls summon them to training exercises, where they practice their skills under conditions like those of a real crisis. For this, they receive about $40 a day on-call pay. The real compensation is in the work itself. It could save lives.

Vital Skills for a Vital Mission

For both ARG and JTOT, the mission is "render safe"—disable the weapon or device before it does any damage—and then move it to a safe spot for disassembly. If a U.S. weapon were involved in an accident, during transport, for example, ARG volunteers would decide how to handle it safely. Los Alamos volunteers are well suited to making that decision because five out of the seven U.S. nuclear weapon systems were developed at Los Alamos. An expert on any one of them would be rapidly available. (For weapons developed by Lawrence Livermore, Livermore designers would serve in the same capacity.)

For ARG, Los Alamos also deploys on-site health and safety personnel, special pneumatic tools for moving a weapon, radiation monitors, and radiographic support in the form of Portac, a portable accelerator. Portac is an x-ray source that can quickly provide high-quality images of a weapon's interior.

Deciphering the mysterious internal workings of a terrorist device would fall to JTOT. Faced with an unknown design, JTOT volunteers would need to evaluate the device, without disturbing or destroying it, and determine how it was put together and what its capabilities might be.

Los Alamos is the lead laboratory for providing the team with nuclear diagnostics—the sensors that detect the types of radiation associated with nuclear weapons and that identify the radiation "signatures" of particular weapon configurations. The "day jobs" of Los Alamos JTOT experts are in programs devoted to developing, testing, and evaluating such tools. So Los Alamos provides JTOT not only with weapon-design experts to deal with a suspected terrorist device but also with the nondestructive evaluation technology they need in the field.

Home Team Backups

Los Alamos JTOT volunteers would not work in isolation at an incident site. They would draw on support from the Home Team, an additional network of Los Alamos and DOE volunteers. The Home Team provides JTOT with rapid access to expanded expertise and programmatic capabilities held ready to meet the needs of those in the field.

The Home Team also provides a vital computing link. At a JTOT incident site, Los Alamos scientists would be able to weigh what their diagnostic tools told them against data from more than a thousand U.S. nuclear tests. Those data are available to them on laptop computers, which would also allow them to run simulations of a device's destructive potential. For more-extensive simulations, they would feed information back to the Home Team, which could tap the Laboratory's computing capability.

All of this work is aimed at providing the military's explosive-ordinance disposal personnel with a workable strategy for disabling a terrorist device and moving it safely away from any population center. "It's a stimulating mental challenge," says one Los Alamos scientist, "although not always fun when you're in a freezing hangar on a NEST exercise. But we volunteer because it's important. Someone has to do it."

NEST volunteers are the ones qualified to do it. ■

Diagnostic tools such as Portac, shown here being used in a training exercise, provide information about a weapon's condition. Portac's x-rays reveal the status of a weapon's high explosives, which, if cracked, must be stabilized with injections of a vulcanizing rubber before the weapon is moved.

Spotlight

Los Alamos in the news

Kevin N. Roark

A silicon wafer is loaded into a small pressure chamber for SCORR processing.

SCORR Wins Presidential Award

A Los Alamos research team is the co-recipient of the top small-business award in the 2002 Presidential Green Chemistry Challenge for its development of SCORR (Supercritical CO_2 Resist Removal). Sponsored by the U.S. Environmental Protection Agency, the award recognizes innovative ways to reduce pollution at its sources. SCORR was cited as a cost-effective, environmentally friendly process that is considered an enabling technology for the semiconductor industry to meet future design goals.

Creating silicon chips is a multistep process in which resist, a polymer film, is used to define circuit patterns through a technique called photolithography. As the circuits are fabricated by etching, excess resist must be removed before the next processing step. SCORR uses carbon dioxide in its supercritical state (possessing the solubility of a liquid and diffusion properties of a gas) as the primary cleaning solvent. Mixed with an environmentally friendly co-solvent, the fluid can penetrate and clean even submicrometer-sized chip features. Returning the carbon dioxide to its gas phase leaves the wafer dry and virtually free of residue; the gas itself can be recycled.

The current industrial process requires hazardous chemicals and as much as six million gallons of water a day at a typical fabrication plant. Environmental and worker safety advocates have criticized both the dangerous solvents and volume of water used. SCORR eliminates these requirements. In addition, as chip features shrink to smaller than 0.13 micrometer, water will not be able to penetrate them because of its relatively high surface tension. The zero surface tension of a supercritical fluid avoids this problem; SCORR thus offers a "green chemistry" approach to cleaning future microchips.

Patented by the Laboratory, the technology is licensed to SC Fluids of Nashua, NH, which is beginning to market it commercially. Los Alamos developers of SCORR are Craig Taylor, Kirk Hollis, Jerry Barton, Leisa Davenhall, Gunilla Jacobson, and Laurie Williams of the Applied Chemical Technology Group and Jim Rubin of the Nuclear Materials Science Group. —*Bill Dupuy*

Metropolis Center Dedicated

The Lab formally dedicated the Nicholas C. Metropolis Center for Modeling and Simulation in late May. The center's two-year construction project ended more than

Presley Salaz

LeRoy N. Sanchez

Opening day at the Nicholas C. Metropolis Center

$13 million under budget and several months ahead of schedule. The center was built to house one of the world's most powerful computers, referred to as the Q.

"This building and the Q supercomputer are essential elements in the National Nuclear Security Administration's Advanced Simulation and Computing program in support of stockpile stewardship," said Laboratory Director John Browne. "This project also demonstrates our commitment to renewing the Lab's infrastructure and ensuring we have the facilities and personnel to fulfill our national security mission. I'm extremely proud of how well our team performed in bringing the construction project to such a successful completion."

The 300,000-square-foot center features a football-field-sized room for the Q, two visualization theaters, five collaboration laboratories, and more than 300 offices plus conference rooms and classrooms. All aspects of its design were aimed at providing the Lab with the latest in support of high-performance computing.

The Q computer is being built by Hewlett Packard; one-third of it has been installed and tested. When fully installed, the Q will be capable of 30 trillion floating-point operations per second, enabling the large-scale computations needed to simulate weapon performance.

Over the center's two-year construction period, the project compiled an enviable safety record. Just a single workday was lost owing to injury out of 600,000 labor hours, and only two recordable injuries occurred, both back strains. More than 1,000 workers were involved in the center's construction. —*Kevin N. Roark*

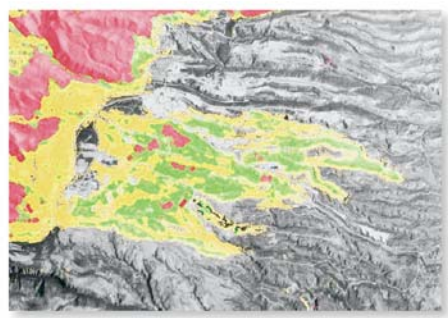
GENIE Wins R&D 100 Award

The Laboratory received an R&D 100 Award for GENIE, a versatile software tool for analyzing digital imagery. The R&D 100 Awards program is an international competition sponsored by *R&D Magazine* that honors the top 100 technological innovations of the year. Winning technologies exemplify the very best in cutting-edge scientific research and development.

GENIE (for Genetic Imagery Exploitation) evolves superior algorithms, or computer codes, for extracting features from images produced by remote-sensing instruments. It is particularly effective in detecting complex features that contain both spatial (shape) and color (wavelength) identifiers, such as wildfire burn scars in satellite images or cancer cells in medical images.

Beginning with a set of low-level image-processing algorithms (for example, edge detectors and spectral operators), GENIE tests each algorithm's ability to identify the feature of interest. The "less fit" algorithms are discarded and the "more fit" ones combined. After many generations of evolution, the resulting algorithm is highly optimized. By automating the algorithm-development process, GENIE will enable fuller analysis of the huge volumes of satellite and other remote-sensing images than is possible with current human and software image analysis.

GENIE was developed by a team of researchers from the Nonproliferation and International Security Division led by Nancy David. —*Brian Fishbine*



GENIE's map of the burn scar from the Cerro Grande wildfire in and around Los Alamos, showing regions of high (red), medium (green), and low (yellow) burn severity.

Mars Odyssey Finds Water

escaping the Martian surface that were generated as a result of cosmic rays striking the planet. The neutrons are emitted in three energy bands: fast, epithermal, and thermal. The energy of these escaping neutrons indicates the degree to which they have been produced and moderated in subsurface nuclear reactions, with both effects related to subsurface composition. Hydrogen is particularly effective in lowering the production and moderating the energy of neutrons, and the relative fluxes of fast, epithermal, and thermal neutrons are strong indicators of near-surface hydrogen.

Modeling that combined the measured neutron fluxes with measured gamma-ray fluxes points to two regions near the poles that are so highly enriched with hydrogen as to require the presence of large reservoirs of near-surface ice. (Gamma-ray emission at 2.2 million electronvolts, an indicator of the capture of thermal neutrons by hydrogen, was also measured.)

The Los Alamos neutron spectrometer will continue to measure neutrons that escape from the top meter of Martian soil for several more years. Scientists will use these data not only to determine the amount of water on Mars but also to map the basaltic lava cover, measure the seasonal variation of polar carbon dioxide frost (dry ice), and help interpret gamma-ray data to determine the quantity and composition of the planet's most abundant elements.

—Shelley Thompson

Researchers Cast "Spiked" Plutonium Alloy

technical lead on the project. The experiment required four years of preparation and included replicating the plutonium manufacturing process that used to be done at the Rocky Flats Plant near Denver, CO. Los Alamos researchers set up a one-of-a-kind, small-scale casting, rolling, and machining operation at TA-55. They also had to reproduce key process steps and produce a material that matched Rocky Flats specifications.

The enriched casting combined plutonium-239 metal that had been "imported" from the Rocky Flats Plant with plutonium-238 metal buttons made at Los Alamos. Fabricating the plutonium-238 buttons was itself a first at TA-55 and a challenge. During casting, every effort was made to duplicate the processing parameters, such as heating and cooling, that were previously used at Rocky Flats.

After casting, the nine spiked ingots were rolled into sheets from which test samples were fabricated. Working with the ingots led to two independent challenges. "First, we had to fabricate the enriched plutonium quickly, because once you make it, it starts aging," said Olivas. "To get time-zero data, we needed to make samples as quickly as possible, and then get them to the test station equally quickly." A twenty-three-day-old sample is about a year old in accelerated time.

The second challenge came from problems associated with the ingots' excess heat from the radioactive decay of plutonium-238. "The ingots started to oxidize within minutes of production, forcing us to conduct all our fabrication operations in a very pristine atmosphere," said Olivas. (Fabrication glove boxes were flushed with argon to minimize the presence of oxygen and moisture.) The extra heat also made taking measurements more difficult. "When we attempted to measure the density of one of the as-cast ingots using the Archimedes method, we boiled the immersion bath fluid," Olivas added.

Initial (time-zero) test results for the spiked plutonium are highly promising. Most of the diagnostic tests show that it behaves very similarly to weapons-grade plutonium in terms of its microstructure, lattice parameters, elastic constants, and dynamic and quasi-static mechanical properties. However, one test, density, is producing anomalous results. Although not yet explained, the anomalies are most likely associated with the presence of the extra plutonium-238.

It is important that the initial material properties of the spiked plutonium be similar to those of weapon plutonium because this is the premise of the study. Having similar results at the outset will allow the aging portion of the study to proceed—and the clock is now ticking.

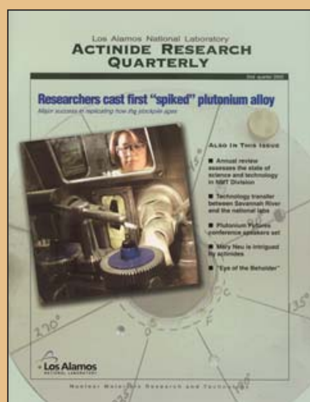
This research is part of the Accelerated Aging of Plutonium Project, an experimental collaboration between Los Alamos and Lawrence Livermore National Laboratories. Scientists at the two labs are conducting parallel sample preparation work and will exchange both information and samples. Their work will be used to predict material and component aging rates as a basis for future decisions about replacing stockpile pits.

—Meredith Coonley

Recent Publications

Science

Research confirming subsurface ice on Mars was featured in the July 5 issue of *Science*. The research is summarized in the Dateline Los Alamos section of this *Quarterly*. (Reprinted with permission from the 5 July 2002 issue of *Science*. Copyright 2002 American Association for the Advancement of Science.)



Susan Carlson

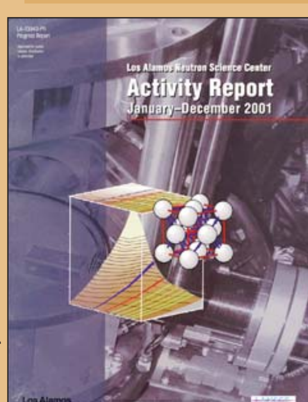
Actinide Research Quarterly

The *Actinide Research Quarterly* highlights current research in the Nuclear Materials Technology Division, focusing on the chemistry, characterization, and analysis of the actinides and on plutonium metallurgy. Current and back issues are available on the Web (http://www.lanl.gov/orgs/nmt/nmtdo/AQarchive/AQhome/AQhome.html).

Gloria Sharp

Los Alamos Science

Issue No. 27 of *Los Alamos Science*—Information, Science, and Technology in a Quantum World—introduces the new field of quantum information science and its application to computing and cryptography. The issue features the Lab's contributions to this field and to topics such as quantum control, decoherence, and single-spin detection. For hard copies or CDs, contact lascience@lanl.gov.



Garth Tietjen

Los Alamos Neutron Science Center Activity Report

The Los Alamos Neutron Science Center Activity Report describes scientific and technological achievements at LANSCE during 2001. LANSCE is an accelerator-based national user facility that generates neutrons for basic and applied research. The report is available on the Web (http://lansce.lanl.gov/libraries/AR2001/AR_2001.htm).